

chain nodes :

30 66 67 68 69 77 78 79 80 81 82 83 84 85 86 87 89

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 31  
 32 33 34 35 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55  
 56 57 58 59 60 61 70 71 72 73 74 75

chain bonds :

30-32 35-89 42-66 48-67 54-68 60-69 66-78 67-79 68-80 69-81 74-77 77-82 78-83  
 79-84 80-85 81-86 82-87

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 13-14 13-18 14-15  
 15-16 16-17 17-18 19-20 19-24 20-21 21-22 22-23 23-24 31-32 31-35 32-33 33-34  
 34-35 38-39 38-43 39-40 40-41 41-42 42-43 44-45 44-49 45-46 46-47 47-48 48-49  
 50-51 50-55 51-52 52-53 53-54 54-55 56-57 56-61 57-58 58-59 59-60 60-61 70-71  
 70-75 71-72 72-73 73-74 74-75

exact/norm bonds :

30-32 31-32 31-35 32-33 33-34 34-35 35-89 42-66 48-67 54-68 60-69 66-78 67-79  
 68-80 69-81 74-77 77-82 78-83 79-84 80-85 81-86 82-87

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 13-14 13-18 14-15  
 15-16 16-17 17-18 19-20 19-24 20-21 21-22 22-23 23-24 38-39 38-43 39-40 40-41  
 41-42 42-43 44-45 44-49 45-46 46-47 47-48 48-49 50-51 50-55 51-52 52-53 53-54  
 54-55 56-57 56-61 57-58 58-59 59-60 60-61 70-71 70-75 71-72 72-73 73-74 74-75

G1: [\*1], [\*2], [\*3], [\*4]

G2: C, N

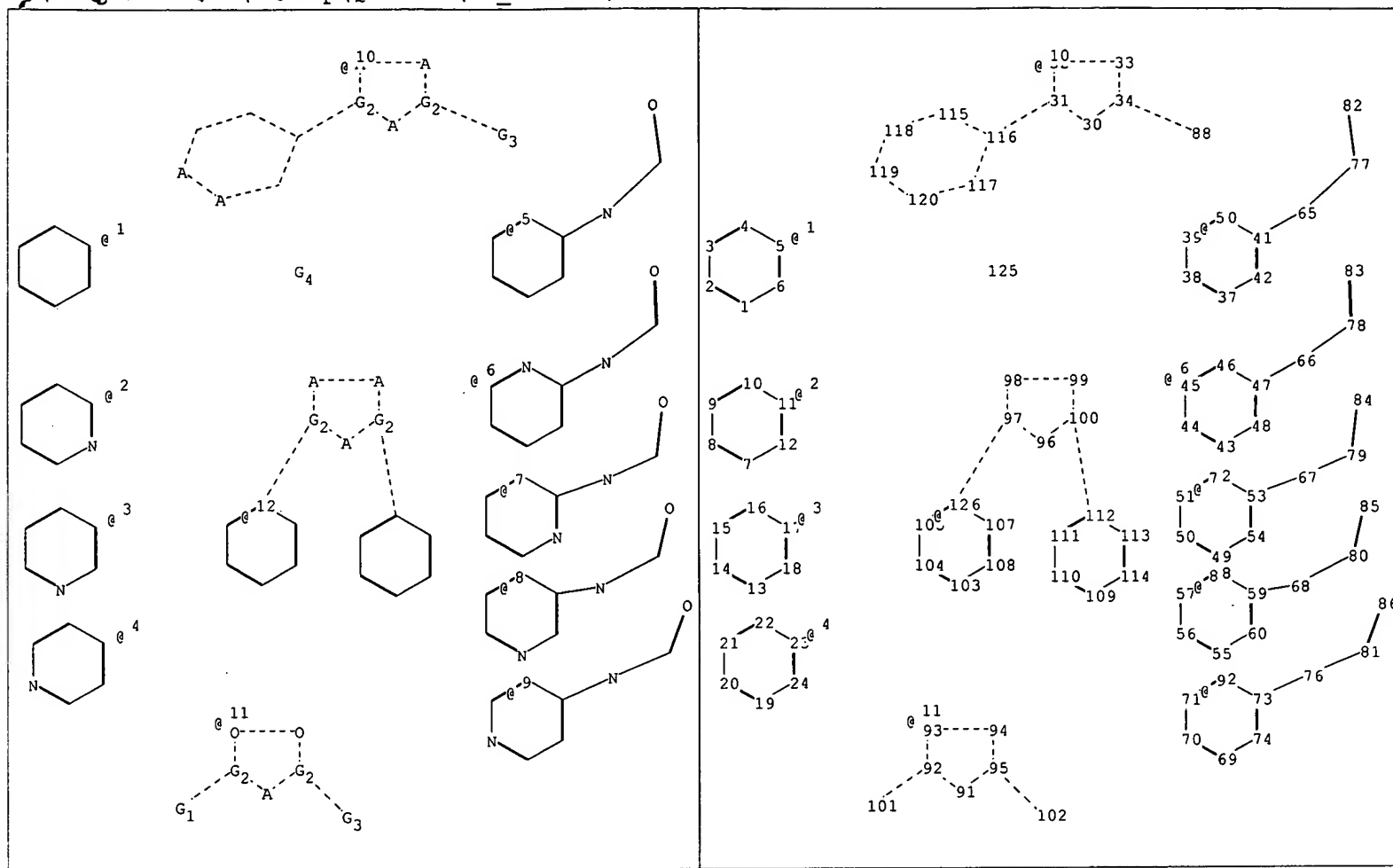
G3: [\*5], [\*6], [\*7], [\*8], [\*9]

Connectivity :

78:3 E exact RC ring/chain 79:3 E exact RC ring/chain 80:3 E exact RC ring/chain  
81:3 E exact RC ring/chain 82:3 E exact RC ring/chain 83:1 E exact RC ring/chain  
84:1 E exact RC ring/chain 85:1 E exact RC ring/chain 86:1 E exact RC ring/chain  
87:1 E exact RC ring/chain

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom  
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom  
22:Atom 23:Atom 24:Atom 30:CLASS 31:Atom 32:Atom 33:Atom 34:Atom 35:Atom 38:Atom  
39:Atom 40:Atom 41:Atom 42:Atom 43:Atom 44:Atom 45:Atom 46:Atom 47:Atom 48:Atom  
49:Atom 50:Atom 51:Atom 52:Atom 53:Atom 54:Atom 55:Atom 56:Atom 57:Atom 58:Atom  
59:Atom 60:Atom 61:Atom 66:CLASS 67:CLASS 68:CLASS 69:CLASS 70:Atom 71:Atom  
72:Atom 73:Atom 74:Atom 75:Atom 77:CLASS 78:CLASS 79:CLASS 80:CLASS 81:CLASS  
82:CLASS 83:CLASS 84:CLASS 85:CLASS 86:CLASS 87:CLASS 89:CLASS



## chain nodes :

65 66 67 68 76 77 78 79 80 81 82 83 84 85 86 88 101 102 125

## ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 30  
 31 32 33 34 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54  
 55 56 57 58 59 60 69 70 71 72 73 74 91 92 93 94 95 96 97 98 99 100  
 103 104 105 106 107 108 109 110 111 112 113 114 115 116 117 118 119 120

## chain bonds :

31-116 34-88 41-65 47-66 53-67 59-68 65-77 66-78 67-79 68-80 73-76 76-81  
 77-82 78-83 79-84 80-85 81-86 92-101 95-102 97-106 100-112

## ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 13-14 13-18 14-15  
 15-16 16-17 17-18 19-20 19-24 20-21 21-22 22-23 23-24 30-31 30-34 31-32 32-33  
 33-34 37-38 37-42 38-39 39-40 40-41 41-42 43-44 43-48 44-45 45-46 46-47 47-48  
 49-50 49-54 50-51 51-52 52-53 53-54 55-56 55-60 56-57 57-58 58-59 59-60 69-70  
 69-74 70-71 71-72 72-73 73-74 91-92 91-95 92-93 93-94 94-95 96-97 96-100  
 97-98 98-99 99-100 103-104 103-108 104-105 105-106 106-107 107-108 109-110  
 109-114 110-111 111-112 112-113 113-114 115-116 115-118 116-117 117-120 118-119  
 119-120

## exact/norm bonds :

30-31 30-34 31-32 31-116 32-33 33-34 34-88 41-65 47-66 53-67 59-68 65-77  
 66-78 67-79 68-80 73-76 76-81 77-82 78-83 79-84 80-85 81-86 91-92 91-95 92-93  
 92-101 93-94 94-95 95-102 96-97 96-100 97-98 97-106 98-99 99-100 100-112  
 115-116 115-118 116-117 117-120 118-119 119-120

## normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 13-14 13-18 14-15  
 15-16 16-17 17-18 19-20 19-24 20-21 21-22 22-23 23-24 37-38 37-42 38-39 39-40  
 40-41



10-646348

# Search history

Davis 10/646348

02/17/2006

=> d his full

(FILE 'HOME' ENTERED AT 09:06:16 ON 17 FEB 2006)

FILE 'STNGUIDE' ENTERED AT 09:06:26 ON 17 FEB 2006

SET LINE 250  
SET DETAIL OFF  
DIS SAVED  
DIS SAVED/S

FILE 'REGISTRY' ENTERED AT 09:06:42 ON 17 FEB 2006

ACT DAV348STRA/A

-----

L1 STR  
L2 ( 4356201)SEA ABB=ON PLU=ON NC5/ESS  
L3 281 SEA SUB=L2 SSS FUL L1

-----  
ACT DAV348STRAX/A

-----

L4 STR  
L5 ( 4356201)SEA ABB=ON PLU=ON NC5/ESS  
L6 ( 281)SEA SUB=L5 SSS FUL L4  
L7 ( 1352901)SEA ABB=ON PLU=ON 46.156.30/RID  
L8 222 SEA ABB=ON PLU=ON L6 AND L7

-----  
SET LINE LOGIN  
SET DETAIL LOGIN

FILE 'STNGUIDE' ENTERED AT 09:06:48 ON 17 FEB 2006

FILE 'REGISTRY' ENTERED AT 09:08:01 ON 17 FEB 2006

L9 195 SEA ABB=ON PLU=ON L8 AND O>1

FILE 'STNGUIDE' ENTERED AT 09:09:29 ON 17 FEB 2006

FILE 'REGISTRY' ENTERED AT 09:36:09 ON 17 FEB 2006

L10 STRUCTURE UPLOADED  
L11 11 SEA SUB=L3 SSS SAM L10  
D SCA  
L12 180 SEA SUB=L3 SSS FUL L10  
SAVE TEMP L12 DAV348NOT1/A  
D SCA L12  
E "CARBAMIC ACID, (3-(5-(3,4-BIS(PHENYLMETHOXY)PHENYL)-1-(2-PY  
L13 1 SEA ABB=ON PLU=ON "CARBAMIC ACID, (3-(5-(3,4-BIS(PHENYLMETHOX  
Y)PHENYL)-1-(2-PYRIDINYL)-1H-PYRAZOL-3-YL)PHENYL)-, PHENYLMETHY  
L ESTER"/CN  
E "BENZAMIDE, N-(4-(2-(2-CHLOROPHENYL)-4-(3-METHYLPHENYL)-5-THI  
L14 1 SEA ABB=ON PLU=ON "BENZAMIDE, N-(4-(2-(2-CHLOROPHENYL)-4-(3-M  
ETHYLPHENYL)-5-THIAZOLYL)-2-PYRIDINYL)-"/CN  
E "BENZENEACETAMIDE, N-(4-(2-(2-CHLOROPHENYL)-4-(3-METHYLPHENYL  
L15 1 SEA ABB=ON PLU=ON "BENZENEACETAMIDE, N-(4-(2-(2-CHLOROPHENYL)  
-4-(3-METHYLPHENYL)-5-THIAZOLYL)-2-PYRIDINYL)-"/CN  
E "BENZENEPROPANAMIDE, N-(4-(2-(2-CHLOROPHENYL)-4-(3-METHYLPHEN  
L16 1 SEA ABB=ON PLU=ON "BENZENEPROPANAMIDE, N-(4-(2-(2-CHLOROPHENY  
L)-4-(3-METHYLPHENYL)-5-THIAZOLYL)-2-PYRIDINYL)-"/CN  
L17 4 SEA ABB=ON PLU=ON (L13 OR L14 OR L15 OR L16)  
SAVE TEMP DAV348ADD/A L17  
L18 101 SEA ABB=ON PLU=ON L3 NOT L12  
L19 105 SEA ABB=ON PLU=ON L18 OR L17

FILE 'CAPLUS' ENTERED AT 10:07:07 ON 17 FEB 2006  
L20 14 SEA ABB=ON PLU=ON L19  
D L1

FILE 'STNGUIDE' ENTERED AT 10:11:08 ON 17 FEB 2006  
D COST

FILE 'REGISTRY' ENTERED AT 10:12:14 ON 17 FEB 2006

FILE 'STNGUIDE' ENTERED AT 10:12:40 ON 17 FEB 2006

FILE 'REGISTRY' ENTERED AT 11:13:29 ON 17 FEB 2006  
L21 ANALYZE PLU=ON L19 1- LC : 4 TERMS  
D

FILE 'USPATFULL' ENTERED AT 11:14:18 ON 17 FEB 2006  
L22 13 SEA ABB=ON PLU=ON L19

FILE 'TOXCENTER' ENTERED AT 11:14:41 ON 17 FEB 2006  
L23 4 SEA ABB=ON PLU=ON L19

FILE 'STNGUIDE' ENTERED AT 11:14:50 ON 17 FEB 2006

FILE 'CAPLUS' ENTERED AT 11:16:05 ON 17 FEB 2006  
E US2003-646348/APPS

L24 10289 SEA ABB=ON PLU=ON SINGH R?/AU  
L25 208 SEA ABB=ON PLU=ON GOFF D?/AU  
L26 396 SEA ABB=ON PLU=ON PARTRIDGE J?/AU  
L27 5 SEA ABB=ON PLU=ON L24 AND L25 AND L26  
L28 9 SEA ABB=ON PLU=ON L24 AND (L25 OR L26)  
L29 5 SEA ABB=ON PLU=ON L25 AND L26

FILE 'USPATFULL' ENTERED AT 11:20:23 ON 17 FEB 2006

L30 565 SEA ABB=ON PLU=ON SINGH R?/AU  
L31 73 SEA ABB=ON PLU=ON GOFF D?/AU  
L32 83 SEA ABB=ON PLU=ON PARTRIDGE J?/AU  
L33 5 SEA ABB=ON PLU=ON L30 AND L31 AND L32  
L34 7 SEA ABB=ON PLU=ON L30 AND (L31 OR L32)  
L35 5 SEA ABB=ON PLU=ON L31 AND L32

FILE 'TOXCENTER' ENTERED AT 11:21:19 ON 17 FEB 2006

L36 2326 SEA ABB=ON PLU=ON SINGH R?/AU  
L37 171 SEA ABB=ON PLU=ON GOFF D?/AU  
L38 101 SEA ABB=ON PLU=ON PARTRIDGE J?/AU  
L39 1 SEA ABB=ON PLU=ON L36 AND L37 AND L38  
L40 2 SEA ABB=ON PLU=ON L36 AND (L37 OR L38)  
L41 1 SEA ABB=ON PLU=ON L37 AND L38  
L42 1 SEA ABB=ON PLU=ON (L39 OR L40 OR L41) AND L23

FILE 'USPATFULL' ENTERED AT 11:22:55 ON 17 FEB 2006

L43 2 SEA ABB=ON PLU=ON (L33 OR L34 OR L35) AND L22  
L44 2 SEA ABB=ON PLU=ON (L30 OR L31 OR L32) AND L22

FILE 'TOXCENTER' ENTERED AT 11:23:44 ON 17 FEB 2006

L45 1 SEA ABB=ON PLU=ON (L36 OR L37 OR L38) AND L23

FILE 'CAPLUS' ENTERED AT 11:24:02 ON 17 FEB 2006

L46 2 SEA ABB=ON PLU=ON (L24 OR L25 OR L26) AND L20

FILE 'STNGUIDE' ENTERED AT 11:25:09 ON 17 FEB 2006

FILE 'REGISTRY' ENTERED AT 11:32:03 ON 17 FEB 2006  
D STAT QUE L19

FILE 'CAPLUS' ENTERED AT 11:32:05 ON 17 FEB 2006

D QUE NOS L27  
D QUE NOS L28  
D QUE NOS L29  
D QUE NOS L46

L47 9 SEA ABB=ON PLU=ON (L27 OR L28 OR L29) OR L46

FILE 'USPATFULL' ENTERED AT 11:32:09 ON 17 FEB 2006

D QUE NOS L33  
D QUE NOS L34  
D QUE NOS L35  
D QUE NOS L43  
D QUE NOS L44

L48 7 SEA ABB=ON PLU=ON (L33 OR L34 OR L35) OR (L43 OR L44)

FILE 'TOXCENTER' ENTERED AT 11:32:13 ON 17 FEB 2006

D QUE NOS L39  
D QUE NOS L40  
D QUE NOS L41  
D QUE NOS L42  
D QUE NOS L45

L49 2 SEA ABB=ON PLU=ON (L39 OR L40 OR L41 OR L42) OR L45

FILE 'STNGUIDE' ENTERED AT 11:32:33 ON 17 FEB 2006

FILE 'CAPLUS, USPATFULL, TOXCENTER' ENTERED AT 11:33:37 ON 17 FEB 2006

L50 15 DUP REM L47 L48 L49 (3 DUPLICATES REMOVED)  
ANSWERS '1-9' FROM FILE CAPLUS  
ANSWERS '10-15' FROM FILE USPATFULL  
D IBIB ABS HITIND HITSTR L50 1-9  
D IBIB ABS HITSTR L50 10-15

FILE 'STNGUIDE' ENTERED AT 11:35:18 ON 17 FEB 2006

FILE 'REGISTRY' ENTERED AT 11:38:43 ON 17 FEB 2006

D STAT QUE L19  
D L21

FILE 'CAPLUS' ENTERED AT 11:38:46 ON 17 FEB 2006

D QUE NOS L20

L51 12 SEA ABB=ON PLU=ON L20 NOT L47

FILE 'USPATFULL' ENTERED AT 11:38:48 ON 17 FEB 2006

D QUE NOS L22

L52 11 SEA ABB=ON PLU=ON L22 NOT L48

FILE 'TOXCENTER' ENTERED AT 11:38:50 ON 17 FEB 2006

D QUE NOS L23

L53 3 SEA ABB=ON PLU=ON L23 NOT L49

FILE 'STNGUIDE' ENTERED AT 11:39:14 ON 17 FEB 2006

FILE 'CAPLUS, USPATFULL, TOXCENTER' ENTERED AT 11:39:50 ON 17 FEB 2006

L54 23 DUP REM L51 L52 L53 (3 DUPLICATES REMOVED)  
ANSWERS '1-12' FROM FILE CAPLUS  
ANSWERS '13-23' FROM FILE USPATFULL

D IBIB ABS HITIND HITSTR L54 1-12  
D IBIB ABS HITSTR L54 13-23

## FILE HOME

## FILE STNGUIDE

FILE CONTAINS CURRENT INFORMATION.

LAST RELOADED: Feb 10, 2006 (20060210/UP).

## FILE REGISTRY

Property values tagged with IC are from the ZIC/VINITI data file  
provided by InfoChem.

STRUCTURE FILE UPDATES: 15 FEB 2006 HIGHEST RN 874326-73-5

DICTIONARY FILE UPDATES: 15 FEB 2006 HIGHEST RN 874326-73-5

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

Please note that search-term pricing does apply when  
conducting SmartSELECT searches.

\*\*\*\*\*  
\*  
\* The CA roles and document type information have been removed from \*  
\* the IDE default display format and the ED field has been added, \*  
\* effective March 20, 2005. A new display format, IDERL, is now \*  
\* available and contains the CA role and document type information. \*  
\*  
\*\*\*\*\*

Structure search iteration limits have been increased. See HELP SLIMITS  
for details.

REGISTRY includes numerically searchable data for experimental and  
predicted properties as well as tags indicating availability of  
experimental property data in the original document. For information  
on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

## FILE CAPLUS

Copyright of the articles to which records in this database refer is  
held by the publishers listed in the PUBLISHER (PB) field (available  
for records published or updated in Chemical Abstracts after December  
26, 1996), unless otherwise indicated in the original publications.  
The CA Lexicon is the copyrighted intellectual property of the  
American Chemical Society and is provided to assist you in searching  
databases on STN. Any dissemination, distribution, copying, or storing  
of this information, without the prior written consent of CAS, is  
strictly prohibited.

FILE COVERS 1907 - 17 Feb 2006 VOL 144 ISS 9

FILE LAST UPDATED: 16 Feb 2006 (20060216/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.  
They are available for your review at:



<http://www.cas.org/infopolicy.html>

FILE USPATFULL

FILE COVERS 1971 TO PATENT PUBLICATION DATE: 16 Feb 2006 (20060216/PD)

FILE LAST UPDATED: 16 Feb 2006 (20060216/ED)

HIGHEST GRANTED PATENT NUMBER: US7000250

HIGHEST APPLICATION PUBLICATION NUMBER: US2006037120

CA INDEXING IS CURRENT THROUGH 14 Feb 2006 (20060214/UPCA)

ISSUE CLASS FIELDS (/INCL) CURRENT THROUGH: 16 Feb 2006 (20060216/PD)

REVISED CLASS FIELDS (/NCL) LAST RELOADED: Dec 2005

USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Dec 2005

FILE TOXCENTER

FILE COVERS 1907 TO 14 Feb 2006 (20060214/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TOXCENTER has been enhanced with new files segments and search fields.  
See HELP CONTENT for more information.

TOXCENTER thesauri in the /CN, /CT, and /MN fields incorporate the  
MeSH 2006 vocabulary.

See <http://www.nlm.nih.gov/mesh/>

[http://www.nlm.nih.gov/pubs/techbull/nd05/nd05\\_med\\_data\\_changes.html](http://www.nlm.nih.gov/pubs/techbull/nd05/nd05_med_data_changes.html)

[http://www.nlm.nih.gov/pubs/techbull/nd05/nd05\\_2006\\_MeSH.html](http://www.nlm.nih.gov/pubs/techbull/nd05/nd05_2006_MeSH.html)

for a description of changes.

=>